## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet V.A1.60 HI60

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This datasheet last evaluated: June 2015; last change in preferred values: June 2015

# $CF_3CF_2CH_2OH + ice \\ CF_3CF_2CF_2CH_2OH + ice \\$

Parameter	Temp./k	K Reference	Technique/ Comments
<i>Partitioning coefficients: K<sub>linC</sub>/cm</i>			
pentafluopropanol-1			
150 ±33	203	Moreno et al., 2012	CWFT-MS (a)
46.4 ±11.6	210		
27.5 ±5	217		
$12.6 \pm 2$	223		
heptafluobutanol-1		Moreno et al., 2012	CWFT-MS (a)
$295 \pm 67$	203		
$108 \pm 36$	210		
$57 \pm 9$	217		
$24.5 \pm 3.4$	223		

## **Experimental data**

### Comments

(a) Uptake of CF<sub>3</sub>CF<sub>2</sub>CH<sub>2</sub>OH (2,2,3,3,3 pentafluopropanol-1) and CF<sub>3</sub>CF<sub>2</sub>CF<sub>2</sub>CH<sub>2</sub>OH (2,2,3,3,4,4,4 heptafluopropanol-1) on a surface film formed by freezing liquid water on inner wall of flow tube. Concentration The adsorption was fully reversible and the data could be described in terms of the Langmuir isotherm over the temperature range 203–223 K. Analysis of the isotherm for gave N<sub>max</sub> = (2.9 ± 0.4) x 10<sup>14</sup> molecule cm<sup>-2</sup> for CF<sub>3</sub>CF<sub>2</sub>CH<sub>2</sub>OH and (3.0 ± 0.5) x 10<sup>14</sup> molecule cm<sup>-2</sup> for CF<sub>3</sub>CF<sub>2</sub>CH<sub>2</sub>OH and (3.0 ± 0.5) x 10<sup>14</sup> molecule cm<sup>-2</sup> for CF<sub>3</sub>CF<sub>2</sub>CF<sub>2</sub>CH<sub>2</sub>OH, independent of temperature. The cited  $K_{\text{linC}}$  values were obtained from the product  $K_{\text{LangC}}(T)$  x N<sub>Max</sub> (=  $K_{\text{linC}}$ ) at each temperature which was within 5% of the slope of the linearised Langmuir plots at the lower concentrations. The temperature dependence of the dimensionless adsorption enthalpy gave  $\Delta H_{\text{ads}} = (-45 \pm 11)$  kJmol<sup>-1</sup> for CF<sub>3</sub>CF<sub>2</sub>CH<sub>2</sub>OH and  $\Delta H_{\text{ads}} = (-46 \pm 16)$  kJmol<sup>-1</sup> for CF<sub>3</sub>CF<sub>2</sub>CF<sub>2</sub>CH<sub>2</sub>OH (error is  $2\sigma + 5\%$ ).

## **Preferred Values**

## CF<sub>3</sub>CF<sub>2</sub>CH<sub>2</sub>OH and CF<sub>3</sub>CF<sub>2</sub>CF<sub>2</sub>CH<sub>2</sub>OH

Parameter	Value	T/K	
$K_{linC}$ / cm	$4.2 \ge 10^{-10} \exp(5390/T)$	203 - 228	
$N_{max}$ / molecule cm <sup>-2</sup>	$2.8 \times 10^{14}$	203 -228	
$K_{linC}$ / cm	$4.2 \ge 10^{-10} \exp(5390/T)$	203 -228	
$N_{max}$ / molecule cm <sup>-2</sup>	$2.8 \times 10^{14}$	203 - 228	

Reliability		
$\Delta(E/R) / K$	$\pm 1000$	200 - 230
$\Delta N_{ m max}$	$\pm 0.5 \text{ x } 10^{14}$	223 - 231

Comments on Preferred Values

The studies of and Moreno et al.(2012a) are the only data reported for the longer chain fluoroalcohols. The uptakes were fully reversible and the Langmuir contants were of similar magnitude to  $CF_3CH_2OH$ , reported in an earlier study (Moreno et al (2012b) on pure ice, which was in agreement with results of Symington et al. (2012). The preferred values accept the values of Moreno et al. (2012).

#### References

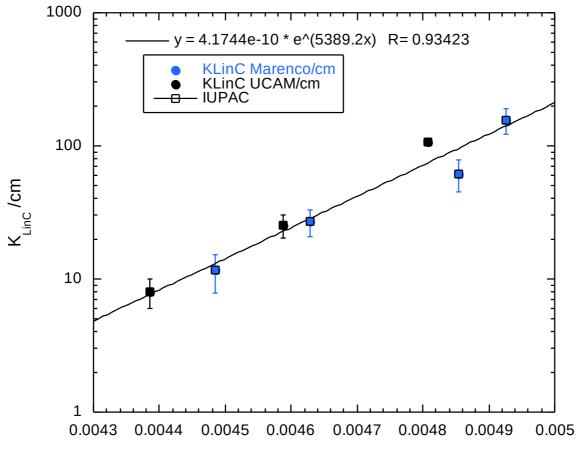
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1/T /K